

=> fil hcaplus
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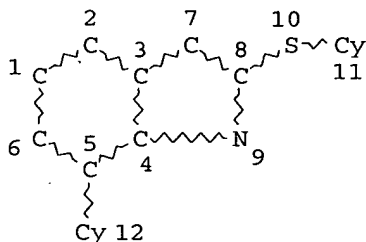
FILE COVERS 1907 - 7 Apr 2006 VOL 144 ISS 16
 FILE LAST UPDATED: 6 Apr 2006 (20060406/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=>
 =>

=> d stat que l13
 L10 STR



NODE ATTRIBUTES:
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 12

STEREO ATTRIBUTES: NONE
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 L13 2 SEA FILE=HCAPLUS ABB=ON PLU=ON L12

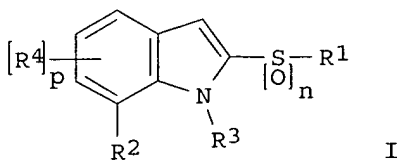
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=> d ibib abs hitstr l13 1-2

L13 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:267299 HCAPLUS
 DOCUMENT NUMBER: 140:303524
 TITLE: Preparation of 2,7-substituted indoles as 5-HT6 modulators
 INVENTOR(S): Madera, Ann Marie; Weikert, Robert James
 PATENT ASSIGNEE(S): F. Hoffmann-La Roche A.-G., Switz.
 SOURCE: PCT Int. Appl., 36 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004026830	A1	20040401	WO 2003-EP10101	20030911
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2496765	AA	20040401	CA 2003-2496765	20030911
AU 2003273855	A1	20040408	AU 2003-273855	20030911
BR 2003014352	A	20050719	BR 2003-14352	20030911
EP 1587788	A1	20051026	EP 2003-757820	20030911
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2006503052	T2	20060126	JP 2004-537044	20030911
US 2004063724	A1	20040401	US 2003-663314	20030916
NO 2005000666	A	20050311	NO 2005-666	20050208
PRIORITY APPLN. INFO.:			US 2002-411239P	P 20020917
OTHER SOURCE(S):			WO 2003-EP10101	W 20030911
GI			MARPAT 140:303524	



AB The title compds. [I; n = 0-2; p = 1-2; R1 = (un)substituted (hetero)aryl; R2 = (un)substituted heterocyclyl; R3 = H, alkyl, COR5 (wherein R5 = alkyl, alkoxy, aryl, aryloxy); R4 = H, OH, CN, alkyl, etc.], useful for treating or preventing a disease state that is alleviated by 5-HT6 agonists, were prepared E.g., a 5-step synthesis of I [n = 2; R1 = Ph; R2 = piperazino; R3 = H; R4 = H], was given. The compds. I were tested and found to have selective 5-HT6 receptor affinity. Activities for representative compds. I were given. The pharmaceutical composition comprising

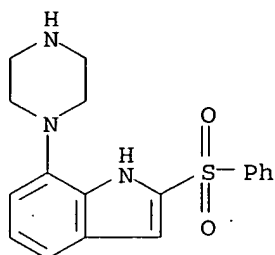
the compound I is claimed.

IT 676446-38-1P 676446-44-9P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of 2,7-substituted indoles as 5-HT6 modulators)

RN 676446-38-1 HCAPLUS

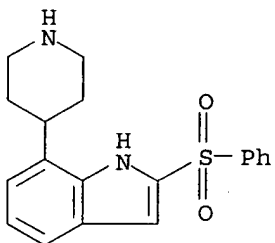
CN 1H-Indole, 2-(phenylsulfonyl)-7-(1-piperazinyl)-, monohydrochloride (9CI)
(CA INDEX NAME)



● HCl

RN 676446-44-9 HCAPLUS

CN 1H-Indole, 2-(phenylsulfonyl)-7-(4-piperidinyl)-, monohydrochloride (9CI)
(CA INDEX NAME)



● HCl

IT 676446-39-2P 676446-40-5P 676446-42-7P

676446-43-8P 676446-45-0P 676446-46-1P

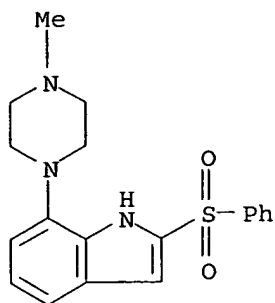
676446-47-2P 676446-48-3P 676446-49-4P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of 2,7-substituted indoles as 5-HT6 modulators)

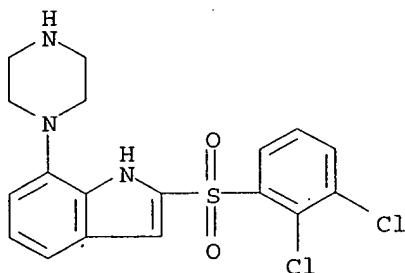
RN 676446-39-2 HCAPLUS

CN 1H-Indole, 7-(4-methyl-1-piperazinyl)-2-(phenylsulfonyl)-, monohydrochloride (9CI) (CA INDEX NAME)



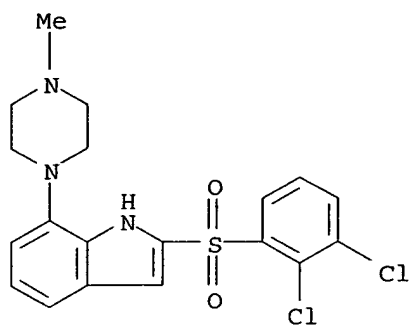
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RN 676446-40-5 HCAPLUS
CN 1H-Indole, 2-[(2,3-dichlorophenyl)sulfonyl]-7-(1-piperazinyl)-,
monohydrochloride (9CI) (CA INDEX NAME)



● HCl

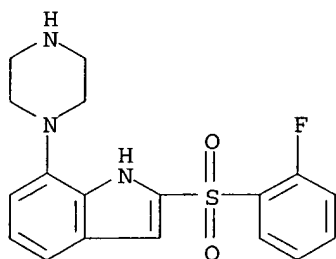
RN 676446-42-7 HCAPLUS
CN 1H-Indole, 2-[(2,3-dichlorophenyl)sulfonyl]-7-(4-methyl-1-piperazinyl)-,
monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 676446-43-8 HCAPLUS

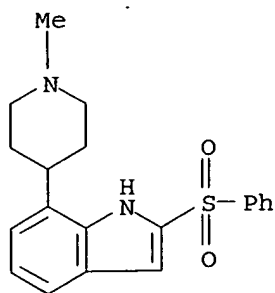
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● HCl

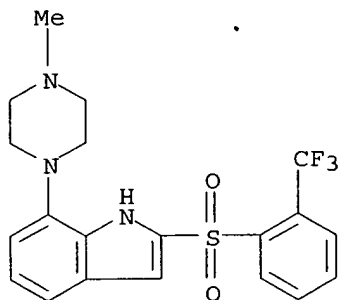
RN 676446-45-0 HCAPLUS

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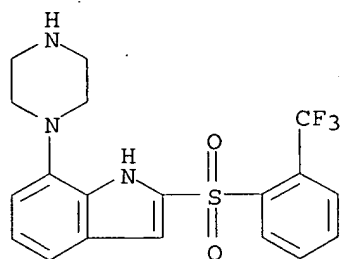


● HCl

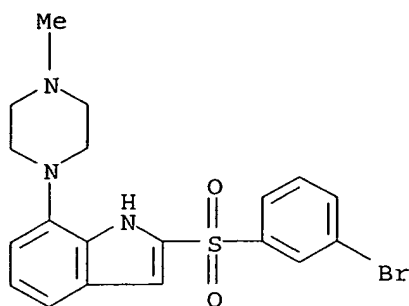
RN 676446-46-1 HCAPLUS
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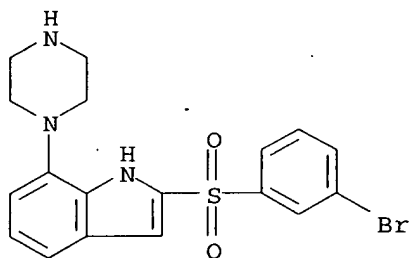
RN 676446-47-2 HCAPLUS
 CN 1H-Indole, 7-(1-piperazinyl)-2-[[2-(trifluoromethyl)phenyl]sulfonyl]- (9CI) (CA INDEX NAME)



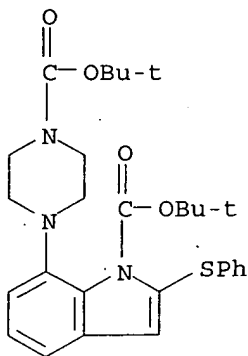
RN 676446-48-3 HCAPLUS
 CN 1H-Indole, 2-[(3-bromophenyl)sulfonyl]-7-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)



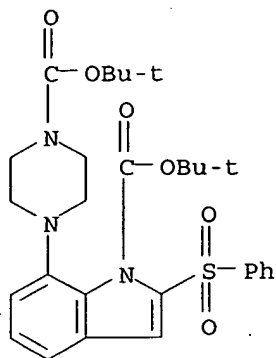
RN 676446-49-4 HCAPLUS
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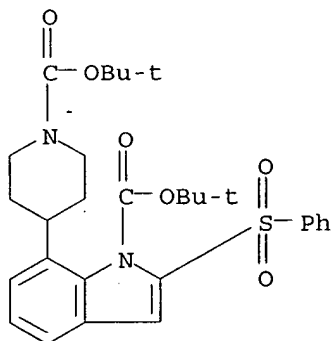
IT 676446-50-7P 676446-51-8P 676446-53-0P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of 2,7-substituted indoles as 5-HT₆ modulators)
 RN 676446-50-7 HCAPLUS
 CN 1H-Indole-1-carboxylic acid, 7-[4-[(1,1-dimethylethoxy)carbonyl]-1-piperazinyl]-2-(phenylthio)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 676446-51-8 HCAPLUS
 CN 1H-Indole-1-carboxylic acid, 7-[4-[(1,1-dimethylethoxy)carbonyl]-1-piperazinyl]-2-(phenylsulfonyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 676446-53-0 HCAPLUS
 CN 1H-Indole-1-carboxylic acid, 7-[1-[(1,1-dimethylethoxy)carbonyl]-4-piperidinyl]-2-(phenylsulfonyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

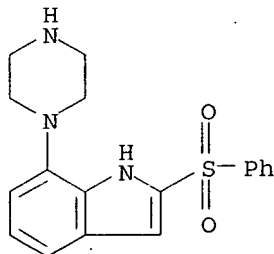


IT 676446-54-1P 676446-55-2P 676446-56-3P
 676446-57-4P 676446-58-5P 676446-59-6P
 676446-60-9P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

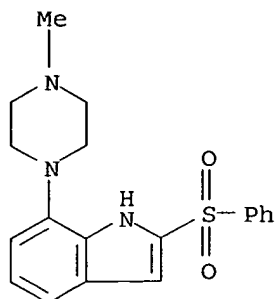
(preparation of 2,7-substituted indoles for treating or preventing a disease state that is alleviated by 5-HT6 agonists)

RN 676446-54-1 HCAPLUS
 CN 1H-Indole, 2-(phenylsulfonyl)-7-(1-piperazinyl)- (9CI) (CA INDEX NAME)



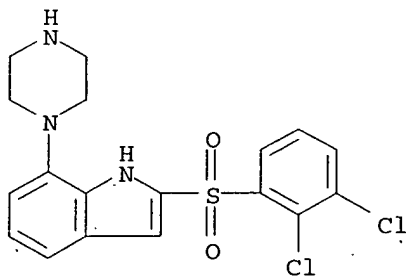
RN 676446-55-2 HCAPLUS

CN 1H-Indole, 7-(4-methyl-1-piperazinyl)-2-(phenylsulfonyl)- (9CI) (CA INDEX NAME)



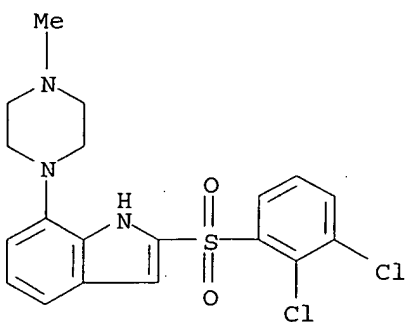
RN 676446-56-3 HCAPLUS

CN 1H-Indole, 2-[(2,3-dichlorophenyl)sulfonyl]-7-(1-piperazinyl)- (9CI) (CA INDEX NAME)



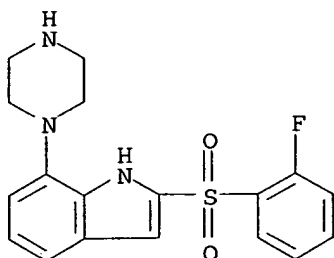
RN 676446-57-4 HCAPLUS

CN 1H-Indole, 2-[(2,3-dichlorophenyl)sulfonyl]-7-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)

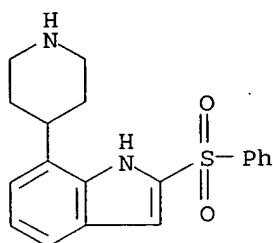


RN 676446-58-5 HCAPLUS

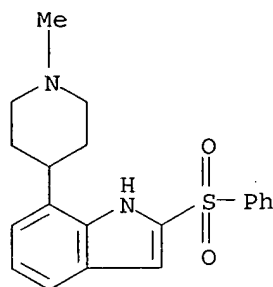
CN 1H-Indole, 2-[(2-fluorophenyl)sulfonyl]-7-(1-piperazinyl)- (9CI) (CA INDEX NAME)



RN 676446-59-6 HCAPLUS
CN 1H-Indole, 2-(phenylsulfonyl)-7-(4-piperidinyl)- (9CI) (CA INDEX NAME)



RN 676446-60-9 HCAPLUS
CN 1H-Indole, 7-(1-methyl-4-piperidinyl)-2-(phenylsulfonyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1996:712944 HCAPLUS
DOCUMENT NUMBER: 126:26455
TITLE: Mechanism of Selective Incorporation of the Melanoma Seeker 2-Thiouracil' into Growing Melanin
AUTHOR(S): Napolitano, Alessandra; Palumbo, Anna; d'Ischia, Marco; Prota, Giuseppe
CORPORATE SOURCE: Department of Organic and Biological Chemistry, University of Naples Federico II, Naples, I-80134, Italy
SOURCE: Journal of Medicinal Chemistry (1996), 39(26), 5192-5201
CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English

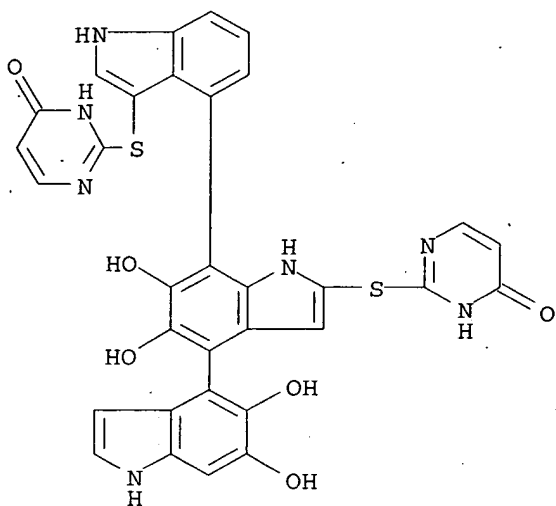
AB The mechanism of selective incorporation of 2-thiouracil (TU), a highly specific melanoma seeker, into growing melanins was investigated both in vitro and in vivo. Methods used included direct anal. of the melanins, by evaluation of the absorption at 350 nm (A350) and chemical degradation coupled with HPLC quantitation of pigment markers, i.e., pyrrole-2,3-dicarboxylic acid (PDCA) and pyrrole-2,3,5-tricarboxylic acid (PTCA), as well as biosynthetic expts. involving tyrosinase-catalyzed oxidation of DOPA, 5,6-dihydroxyindole (DHI), and 5,6-dihydroxyindole-2-carboxylic acid (DHICA). Injection of radiolabeled TU into melanoma-bearing mice resulted in a rapid incorporation of the drug into the tumor pigment, with a substantial decrease in A350 and in PTCA yields. Similar changes in the absorption properties were observed in biosynthetic melanins prepared in the presence of TU, whereas the yields of PTCA and PDCA varied depending on the pigment precursor used. When incubated with DOPA in the presence of tyrosinase, TU profoundly modified the normal course of melanogenesis, favoring formation of a complex mixture of addition products consisting mainly of 6-S-thiouracil-DOPA as well as DHI-TU adducts. The latter were obtained in larger amts. by enzymic oxidation of DHI in the presence of TU and were identified as the 3- and 2-substituted adducts, the dimer, and the trimer. Similar reactions carried out on DHICA yielded the 4-substituted adduct, the dimer, and the trimer. A new mechanistic scheme for the incorporation of TU into growing melanin is proposed, which envisages nucleophilic attack of the thioureylene moiety of TU to transient quinonoid intermediates in the melanin pathway, chiefly dopaquinone and 5,6-indolequinones, followed by entrainment of the resulting adducts into the growing pigment via oxidative copolymn. with DHICA and/or DHI.

IT 184846-17-1P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (mechanism of selective incorporation of melanoma seeker 2-thiouracil into growing melanin)

RN 184846-17-1 HCAPLUS

CN 4(1H)-Pyrimidinone, 2,2'-[(5,5',6,6'-tetrahydroxy[4,4':7',4''-ter-1H-indole]-2',3''-diyl)bis(thio)]bis- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

44

THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> => fil beil

FILE 'BEILSTEIN' ENTERED AT 16:32:52 ON 07 APR 2006

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FILE LAST UPDATED ON MARCH 15, 2006

FILE COVERS 1771 TO 2006.

*** FILE CONTAINS 9,516,393 SUBSTANCES ***

>>>PLEASE NOTE: Reaction Data and substance data are stored in separate documents and can not be searched together in one query. Reaction data for BEILSTEIN compounds may be displayed immediately with the display codes PRE (preparations) and REA (reactions). A substance answer set retrieved after the search for a chemical name, a compounds with available reaction information by combining with PRE/FA, REA/FA or more generally with RX/FA. The BEILSTEIN Registry Number (BRN) is the link between a BEILSTEIN compound and belonging reactions. For more detailed reaction searches BRNs can be searched as reaction partner BRNs Reactant BRN (RX.RBRN) or Product BRN (RX.PBRN).<<<

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 * SET NOTICE FEATURE: THE COST ESTIMATES CALCULATED FOR SET NOTICE *
 * ARE BASED ON THE HIGHEST PRICE CATEGORY. THEREFORE; THESE *
 * ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS. *
 * FOR PRICE INFORMATION SEE HELP COST *

NEW

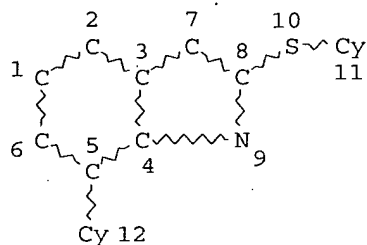
* PATENT NUMBERS (PN) AND BABS ACCESSION NUMBERS (BABSAN) CAN NOW BE SEARCHED, SELECTED AND TRANSFERRED.
 * NEW DISPLAY FORMATS ALLREF, ALLP AND BABSAN SHOW ALL REFERENCES, ALL PATENT REFERENCES, OR ALL BABS ACCESSION NUMBERS FOR A COMPOUND AT A GLANCE.

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=> d stat que 115

L10 STR



NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 12

STEREO ATTRIBUTES: NONE

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L14 1 SEA FILE=BEILSTEIN SSS FUL L10
L15 1 SEA FILE=BEILSTEIN ABB=ON PLU=ON L14 NOT L12

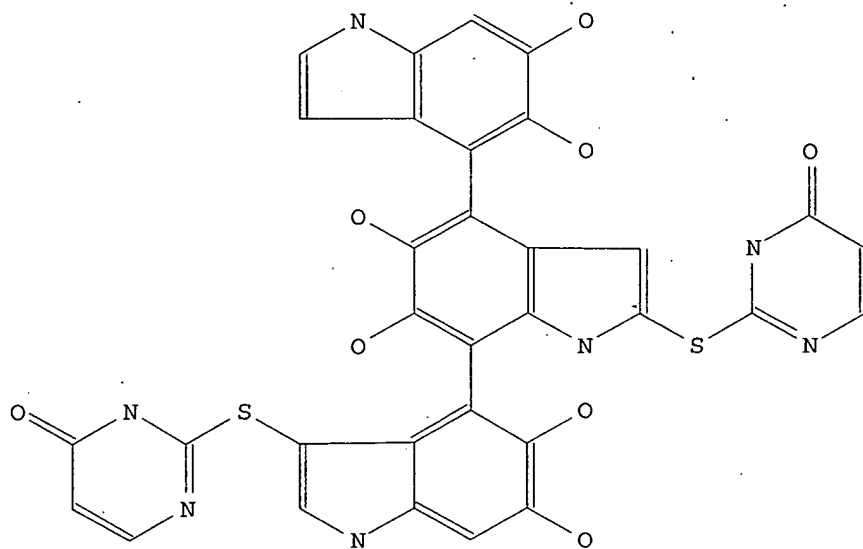
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L15 ANSWER 1 OF 1 BEILSTEIN COPYRIGHT 2006 BEILSTEIN MDL on STN

Beilstein Records (BRN):	7681091
Chemical Name (CN):	5,5',5'',6,6',6''-hexahydroxy-2',3-bis<(4-hydroxypyrimidin-2-yl)thio>4,7':4',4''-terindolyl
Molecular Formula (MF):	C32 H21 N7 O8 S2
Molecular Weight (MW):	695.68
Beilstein Citation (BSO):	6-26



Reaction:
RX

Reaction ID (.ID):	4607437
Reactant BRN (.RBRN):	122055, 112227
Reactant (.RCT):	indole-5,6-diol, 2-thioxo-2,3-dihydro-1H-pyrimidin-4-one
Product BRN (.PBRN):	7651201, 7676466, 7681091, 7649479

Product (.PRO): 2-(5,6-dihydroxy-1H-indol-3-ylsulfanyl)-3H-pyrimidin-4-one, 5,5',6,6'-tetrahydroxy-2,2'-bis<(4-hydroxypyrimidin-2-yl)thio>-4,4'-biindolyl, 5,5',5'',6,6',6''-hexahydroxy-2',3-bis<(4-hydroxypyrimidin-2-yl)thio>4,7':4',4''-terindolyl, 2-(5,6-dihydroxy-1H-indol-2-ylsulfanyl)-3H-pyrimidin-4-one

No. of React. Details (.NVAR): 5

Reaction Details:

RX

Reaction RID (.RID): 4607437.1
Reaction Classification (.CL): Preparation
Yield (.YDT): 4 percent (BRN=7649479), 5 percent (BRN=7651201), 2 percent (BRN=7676466), 9 percent (BRN=7681091)
Reagent (.RGT): phosphate buffer pH 7.0, mushroom tyrosinase
Time (.TIM): 50 min
Reference(s):
1. Napolitano, Alessandra; Palumbo, Anna; d'Ischia, Marco; Prota, Giuseppe, J.Med.Chem., CODEN: JMCMAR, 39(26), <1996>, 5192-5201; BABS-6049529

RX

Reaction RID (.RID): 4607437.2
Reaction Classification (.CL): Preparation
Yield (.YDT): 5 percent (BRN=7651201), 4 percent (BRN=7649479), 2 percent (BRN=7676466), 9 percent (BRN=7681091)
Reagent (.RGT): phosphate buffer pH 7.0, mushroom tyrosinase
Time (.TIM): 50 min
Reference(s):
1. Napolitano, Alessandra; Palumbo, Anna; d'Ischia, Marco; Prota, Giuseppe, J.Med.Chem., CODEN: JMCMAR, 39(26), <1996>, 5192-5201; BABS-6049529

RX

Reaction RID (.RID): 4607437.3
Reaction Classification (.CL): Preparation
Yield (.YDT): 9 percent (BRN=7681091), 5 percent (BRN=7651201), 4 percent (BRN=7649479), 2 percent (BRN=7676466)
Reagent (.RGT): phosphate buffer pH 7.0, mushroom tyrosinase
Time (.TIM): 50 min
Reference(s):
1. Napolitano, Alessandra; Palumbo, Anna; d'Ischia, Marco; Prota, Giuseppe, J.Med.Chem., CODEN: JMCMAR, 39(26), <1996>, 5192-5201; BABS-6049529

RX

Reaction RID (.RID): 4607437.4
Reaction Classification (.CL): Preparation
Yield (.YDT): 2 percent (BRN=7676466), 5 percent (BRN=7651201), 4 percent (BRN=7649479), 9 percent (BRN=7681091)
Reagent (.RGT): phosphate buffer pH 7.0, mushroom tyrosinase
Time (.TIM): 50 min
Reference(s):

1. Napolitano, Alessandra; Palumbo, Anna; d'Ischia, Marco; Prota, Giuseppe, J.Med.Chem., CODEN: JMCMAR, 39(26), <1996>, 5192-5201; BABS-6049529

RX

Reaction RID (.RID): 4607437.5
 Reaction Classification (.CL): Chemical behaviour
 Yield (.YDT): 5 percent (BRN=7651201), 4 percent (BRN=7649479), 2 percent (BRN=7676466), 9 percent (BRN=7681091)
 Reagent (.RGT): phosphate buffer pH 7.0, mushroom tyrosinase
 Time (.TIM): 50 min
 Other Conditions (.COND): other melanin precursor
 Subject Studied (.SUBJ): Product distribution, Mechanism
 Reference(s):
 1. Napolitano, Alessandra; Palumbo, Anna; d'Ischia, Marco; Prota, Giuseppe, J.Med.Chem., CODEN: JMCMAR, 39(26), <1996>, 5192-5201; BABS-6049529

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FILE 'HCAPLUS' ENTERED AT 16:33:55 ON 07 APR 2006

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FILE COVERS 1907 - 7 Apr 2006 VOL 144 ISS 16

FILE LAST UPDATED: 6 Apr 2006 (20060406/ED)

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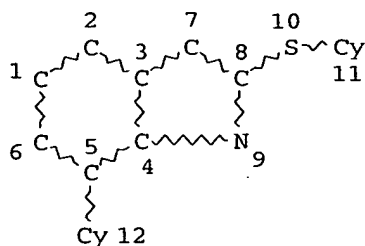
This file contains CAS Registry Numbers for easy and accurate substance identification.

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L10 STR



NODE ATTRIBUTES:
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 12

STEREO ATTRIBUTES: NONE

L12 22 SEA FILE=REGISTRY SSS FUL L10
 L13 2 SEA FILE=HCAPLUS ABB=ON PLU=ON L12
 L16 7 SEA FILE=HCAPLUS ABB=ON PLU=ON "MADERA A"/AU OR "MADERA ANN
 MARIE"/AU
 L17 6 SEA FILE=HCAPLUS ABB=ON PLU=ON L16 NOT L13

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L17 ANSWER 1 OF 6 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:267300 HCAPLUS

DOCUMENT NUMBER: 140:303525

TITLE: Preparation of 2,4-substituted indoles as 5-HT6
 modulators

INVENTOR(S): Madera, Ann Marie; Weikert, Robert James

PATENT ASSIGNEE(S): F. Hoffmann-La Roche A.-G., Switz.

SOURCE: PCT Int. Appl., 38 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

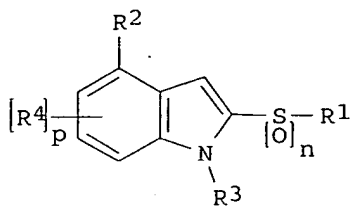
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004026831	A1	20040401	WO 2003-EP9969	20030908
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
CA 2498946	AA	20040401	CA 2003-2498946	20030908
AU 2003267063	A1	20040408	AU 2003-267063	20030908
EP 1542973	A1	20050622	EP 2003-747986	20030908

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK

BR 2003014363	A	20050719	BR 2003-14363	20030908
JP 2006502177	T2	20060119	JP 2004-537019	20030908
US 2004072844	A1	20040415	US 2003-663335	20030916
NO 2005000664	A	20050415	NO 2005-664	20050208

PRIORITY APPLN. INFO.:		US 2002-411480P	P	20020917
		WO 2003-EP9969	W	20030908

OTHER SOURCE(S): MARPAT 140:303525
GI



AB The title compds. [I; n = 0-2; p = 1-2; R1 = (un)substituted (hetero)aryl; R2 = (un)substituted heterocyclyl; R3 = H, alkyl, COR5 (wherein R5 = alkyl, alkoxy, aryl, aryloxy); R4 = H, OH, CN, alkyl, etc.], useful for treating or preventing a disease state that is alleviated by 5-HT6 agonists; were prepared E.g., a 3-step synthesis of I [n = 2; R1 = 2-FC6H4; R2 = piperazino; R3, R4 = H], was given. The compds. I were tested and found to have selective 5-HT6 receptor affinity. Activities for representative compds. I were given. The pharmaceutical composition comprising the compound I is claimed.

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 2 OF 6 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:915299 HCAPLUS

DOCUMENT NUMBER: 140:111370

TITLE: Synthesis of vinylsulfonamides using the Horner reaction

AUTHOR(S): Reuter, Deborah C.; McIntosh, Joel E.; Guinn, Ashley C.; Madera, Ann Marie

CORPORATE SOURCE: Department of Medicinal Chemistry, Roche Palo Alto, Palo Alto, CA, 94304, USA

SOURCE: Synthesis (2003), (15), 2321-2324
CODEN: SYNTBF; ISSN: 0039-7881

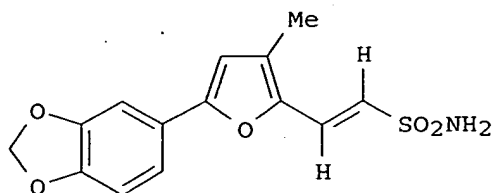
PUBLISHER: Georg Thieme Verlag

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 140:111370

GI



AB A series of vinylsulfonamides, e.g., I, was synthesized using the Horner reaction of aldehydes with diphenylphosphorylmethanesulfonamide. The sulfonamide reagent was easily prepared and can be stored indefinitely. The trans orientation about the double bond of the vinyl sulfonamides was the only isomer observed

REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 3 OF 6 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:454291 HCAPLUS

DOCUMENT NUMBER: 139:22114

TITLE: Preparation of aminotetralin derivatives as muscarinic receptor antagonists

INVENTOR(S): Madera, Ann Marie; Weikert, Robert James

PATENT ASSIGNEE(S): F. Hoffmann-La Roche AG, Switz.

SOURCE: PCT Int. Appl., 57 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

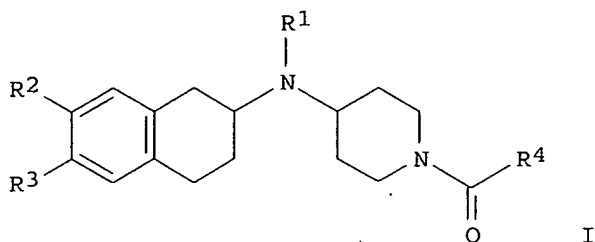
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

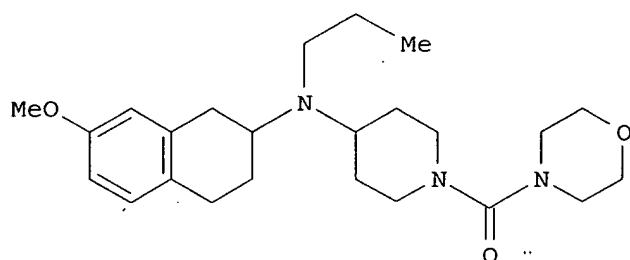
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003048125	A1	20030612	WO 2002-EP13219	20021125
W:			AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW	
RW:			GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG	
CA 2469055	AA	20030612	CA 2002-2469055	20021125
AU 2002352124	A1	20030617	AU 2002-352124	20021125
EP 1453806	A1	20040908	EP 2002-787797	20021125
R:			AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK	
BR 2002014649	A	20041103	BR 2002-14649	20021125
JP 2005518368	T2	20050623	JP 2003-549317	20021125
CN 1639124	A	20050713	CN 2002-824017	20021125
US 2003171362	A1	20030911	US 2002-308092	20021202
US 6635658	B2	20031021		
US 2004092604	A1	20040513	US 2003-608604	20030627
US 6806278	B2	20041019		
PRIORITY APPLN. INFO.:			US 2001-336675P	P 20011203
			WO 2002-EP13219	W 20021125

OTHER SOURCE(S):
GI

MARPAT 139:22114



I



II

AB Title compds. I [] are prepared For instance, 7-methoxy-3,4-dihydro-1H-naphthalen-2-one is alkylated with [1-benzylpiperidin-4-yl]amine (ClCH₂CH₂Cl, NaHB(OAc)₃), the resulting product is alkylated with propionaldehyde (ClCH₂CH₂Cl, NaHB(OAc)₃), debenzylated (EtOH, H₂-Pd(OH)₂) and acylated with morpholine-4-carbonyl chloride (CH₂Cl₂, DIEA) to give II. II has pK_i = 8.57 and 8.83 for the muscarinic M₂ and M₃ receptor resp. I are useful for the treatment of smooth muscle disorders and genitourinary diseases.

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 4 OF 6 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:454290 HCAPLUS

DOCUMENT NUMBER: 139:36440

TITLE: Preparation of 4-piperidinyl alkylamine derivatives as muscarinic receptor antagonists

INVENTOR(S): Brotherton-Pleiss, Christine E.; Madera, Ann Marie; Weikert, Robert James

PATENT ASSIGNEE(S): F. Hoffmann-La Roche Ag, Switz.

SOURCE: PCT Int. Appl., 86 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.

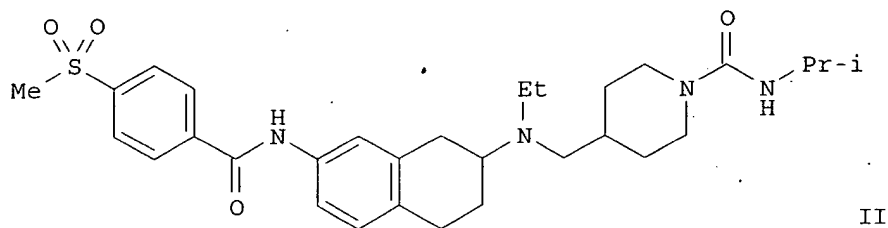
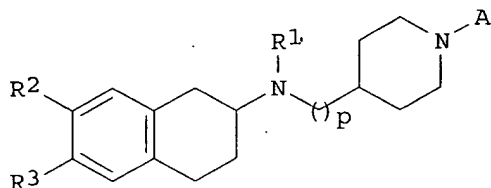
KIND

DATE

APPLICATION NO.

DATE

WO 2003048124	A1	20030612	WO 2002-EP13220	20021125
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2468691	AA	20030612	CA 2002-2468691	20021125
AU 2002352125	A1	20030617	AU 2002-352125	20021125
EP 1453805	A1	20040908	EP 2002-787798	20021125
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
BR 2002014674	A	20041019	BR 2002-14674	20021125
JP 2005517641	T2	20050616	JP 2003-549316	20021125
US 2003162780	A1	20030828	US 2002-308081	20021202
US 6627644	B2	20030930		
US 2004092554	A1	20040513	US 2003-611193	20030701
US 6864266	B2	20050308		
PRIORITY APPLN. INFO.:			US 2001-336795P	P 20011203
			WO 2002-EP13220	W 20021125
			US 2002-308081	A1 20021202
OTHER SOURCE(S):				
GI			MARPAT 139:36440	



AB Title compds. I [A = acyl, sulfonyl; R1 = alkyl, allyl; R2-3 = H, halo, (hetero)aryl, etc.; p = 1-2] are prepared For instance, 7-nitro-3,4-dihydro-1H-naphthalen-2-one is used to alkylate 4-(aminomethyl)piperidine-1-carboxylic acid tert-Bu ester (1,2-dichloroethane, NaHB(OAc)3), the product alkylated with acetaldehyde

(1,2-dichloroethane, NaHB(OAc)₃), reduced (EtOH, H₂-Pd/C) to the corresponding aniline, acylated with 4-(methanesulfonyl)benzoyl chloride (EtOAc, K₂CO₃), deprotected (CH₂Cl₂, TFA) and treated with isopropylisocyanate (CH₂Cl₂) to give II. Muscarinic M₂/M₃ inhibitory activities are determined for selected compds. I are useful for the treatment of genitourinary disorders.

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 5 OF 6 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:868428 HCAPLUS

DOCUMENT NUMBER: 136:6017

TITLE: Substituted 1-aminoalkyl-lactams and their use as muscarinic receptor antagonists

INVENTOR(S): Madera, Ann Marie; Stabler, Russell Stephen; Weikert, Robert James

PATENT ASSIGNEE(S): F. Hoffmann-La Roche A.-G., Switz.

SOURCE: PCT Int. Appl., 69 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

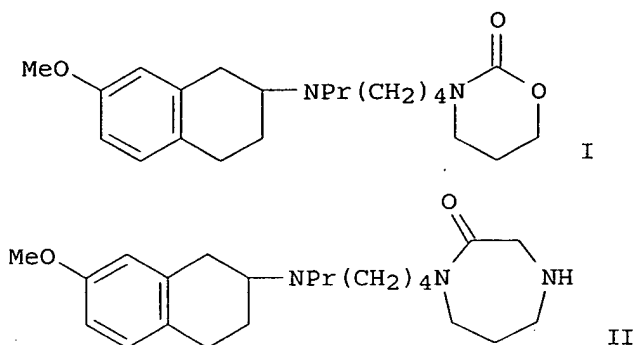
FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001090082	A1	20011129	WO 2001-EP5631	20010517
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CA 2408934	AA	20011129	CA 2001-2408934	20010517
EP 1289964	A1	20030312	EP 2001-933980	20010517
EP 1289964	B1	20041020		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
BR 2001011019	A	20030617	BR 2001-11019	20010517
JP 2003534331	T2	20031118	JP 2001-586271	20010517
NZ 522410	A	20040924	NZ 2001-522410	20010517
AT 280162	E	20041115	AT 2001-933980	20010517
RU 2243222	C2	20041227	RU 2002-133220	20010517
ES 2230310	T3	20050501	ES 2001-1933980	20010517
US 2002004494	A1	20020110	US 2001-862522	20010522
US 6500822	B2	20021231		
ZA 2002008895	A	20040219	ZA 2002-8895	20021101
US 2003109524	A1	20030612	US 2002-289055	20021106
US 6645958	B2	20031111		
ZA 2002009029	A	20040206	ZA 2002-9029	20021106
NO 2002005641	A	20021217	NO 2002-5641	20021122
US 2004034018	A1	20040219	US 2003-632734	20030801
US 6818645	B2	20041116		
US 2004087581	A1	20040506	US 2003-685124	20031014
PRIORITY APPLN. INFO.:			US 2000-207483P	P 20000525
			US 2001-267617P	P 20010209
			US 2001-267579P	P 20010209
			WO 2001-EP5631	W 20010517

US 2001-862286	A3 20010522
US 2001-862522	A3 20010522
US 2002-289055	A3 20021106

OTHER SOURCE(S): MARPAT 136:6017
GI



AB Title compds. such as I and II were prepared Thus, I was prepared in two steps from 3,4-dihydro-7-methoxy-2(1H)-naphthalenone and PrNH₂. Muscarinic inhibitory activities (expressed as pK_i values) of I were 8.20 (m2), 7.56 (m3), 6.30 (m5).

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 6 OF 6 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2000:70963 HCAPLUS

DOCUMENT NUMBER: 132:225007

TITLE: Geology, alteration and mineralization of the Tampakan copper deposit, Philippines

AUTHOR(S): Rohrlach, B.; Madera, A.; Watt, R.

CORPORATE SOURCE: Research School of Earth Sciences, Canberra, 2617, Australia

SOURCE: Publications of the Australasian Institute of Mining and Metallurgy (1999), 4/99(PACRIM '99 Congress, 1999), 517-525

CODEN: AIMMEM; ISSN: 1324-6240

PUBLISHER: Australasian Institute of Mining and Metallurgy

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The Tampakan deposit is a strongly telescoped high-sulfidation-epithermal/porphyry deposit pair which is hosted by a sequence of probable Pliocene age subaerial andesite flows. These host units lie on the western flank of a deeply dissected andesitic stratovolcano within the northernmost portion of the Sangihe Arc in southern Mindanao. The deposit was discovered in 1992 and is currently undergoing resource evaluation. Preliminary resource estns. indicate a total inferred metal content of 12 million tonnes of copper metal and 16 million oz of gold. Using a 0.2 per cent Cu cut-off grade, the deposit has a current mineral resource of approx. 2.5 billion tonnes with an estimated grade of 0.48 per cent copper. At a higher cut-off grade of 0.5 per cent Cu, the mineral resource is approx. 900 million tonnes with an estimated grade of 0.75 per cent copper. Mineralization is open both to the west and at depth. The Tampakan district is centrally located with respect to a 100 km wide zone of

L13 2 SEA FILE=HCAPLUS ABB=ON PLU=ON L12
 L16 7 SEA FILE=HCAPLUS ABB=ON PLU=ON "MADERA A"/AU OR "MADERA ANN
 MARIE"/AU
 L17 6 SEA FILE=HCAPLUS ABB=ON PLU=ON L16 NOT L13
 L18 18 SEA FILE=HCAPLUS ABB=ON PLU=ON ("WEIKERT R M"/AU OR "WEIKERT
 ROBERT J"/AU OR "WEIKERT ROBERT JAMES"/AU)
 L19 13 SEA FILE=HCAPLUS ABB=ON PLU=ON L18 NOT (L13 OR L17)

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=> d ibib abs hitstr l19 1-13

L19 ANSWER 1 OF 13 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:1313863 HCAPLUS

DOCUMENT NUMBER: 144:51448

TITLE: Preparation of 3-amino-1-arylpropylindoles as
monoamine reuptake inhibitors for depressionINVENTOR(S): Greenhouse, Robert; Jaime-Figueroa, Saul; Raptova,
Lubica; Reuter, Deborah Carol; Stein, Karin Ann;
Weikert, Robert James

PATENT ASSIGNEE(S): F.Hoffmann-La Roche AG, Switz.

SOURCE: PCT Int. Appl., 126 pp.

CODEN: PIXXD2

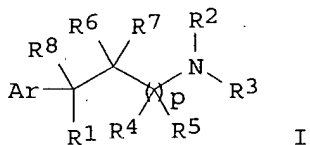
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005118539	A1	20051215	WO 2005-EP5734	20050527
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2006025467	A1	20060202	US 2005-142076	20050601
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OTHER SOURCE(S):			MARPAT 144:51448	
GI				

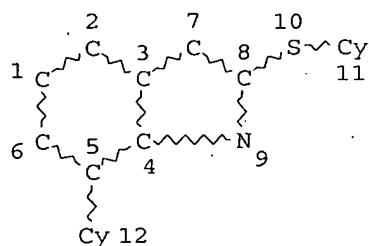


AB Title compds. I [p = 1-2; Ar = (un)substituted (un)saturated indolyl,

left-lateral strike-slip deformation represented by the trans-Mindanao Cotabato Fault Zone. The district is transected by several WNW-striking wrench faults which represent strands of the regional Cotabato Fault Zone. High-sulfidation epithermal mineralization within the Tampakan deposit is strongly controlled by NNE-trending faults which lie along a dilational orientation within the Pliocene stress field associated with the Cotabato strike-slip fault zone. The mineralization is broadly hosted by a gently-dipping, tabular zone of partial to massive silicification which displays multi-phase brecciation, acid-leaching, related vuggy porosity and which is developed within a district-scale advanced-argillic and argillic litho-cap exceeding 90 km² in area. High-sulfidation epithermal mineralization is associated with silica-pyrophyllite-dickite-alunite-diaspore-sericite alteration assemblage which is transitional downward to sericite-chlorite alteration and relict potassic biotite-chlorite-magnetite-anhydrite alteration associated with pervasively developed but weakly mineralized porphyry quartz stockwork veins. The high-sulfidation mineralization is dominated by disseminated, vein and vug-filling enargite-bornite-digenite-chalcocite-covellite ± molybdenite which has overprinted an earlier phase of porphyry copper stockwork veins associated with high-level porphyritic hornblende diorite stocks. The distribution of high-sulfidation alteration and mineralization reflects strong stratigraphic and structural controls. The high-sulfidation mineralization covers a surface area of approx. 1.6 km by 2.0 km and forms a tabular, flat-lying to gently-dipping body between 200 and 500 m thick. It is intersected at RL-1200 m ASL (at surface) in the northern portion of the deposit and extends down to RL-600 m ASL at the southern end. The deposit has been diamond-drill tested to a depth of 400 - 500 m where low-grade chalcopyrite-bornite-pyrite mineralization is hosted by pervasive quartz stockwork veins. This deep-level mineralization represents the outer portion of a porphyry Cu system hosted by both andesite flows and the uppermost portions of high-level hornblende diorite stocks. Deep drilling to test for higher tenor porphyry Cu mineralization is planned.

REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L10 STR



NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 12

STEREO ATTRIBUTES: NONE
L12 22 SEA FILE=REGISTRY SSS FUL L10

benzimidazolyl, etc.; R1 = Ph, naphthyl, etc.; R2-3 = H, alkyl, hydroxyalkyl, etc.; R6 = H, alkyl, etc.; R7 = H, alkyl, OH, alkoxy, hydroxyalkyl, etc.; R4-5 = H, alkyl, etc.] are prepared. For instance, [3-(1H-indol-3-yl)-3-phenylpropyl]methylamine (II) is prepared in 3 steps from indole, Meldrum's acid and benzaldehyde. II has a pKi = 8.45 for the human serotonin reuptake transporter. I are useful for the treatment of depression and anxiety.

REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 2 OF 13 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1999:207703 HCAPLUS

DOCUMENT NUMBER: 130:337878

TITLE: Synthesis of Mexiletine Stereoisomers and Related Compounds via SNAr Nucleophilic Substitution of a Cr(CO)₃-Complexed Aromatic Fluoride

AUTHOR(S): Loughhead, David G.; Flippin, Lee A.; Weikert, Robert J.

CORPORATE SOURCE: Department of Medicinal Chemistry Neurobiology Unit, Roche Bioscience, Palo Alto, CA, 94304, USA

SOURCE: Journal of Organic Chemistry (1999), 64(9), 3373-3375
CODEN: JOCEAH; ISSN: 0022-3263

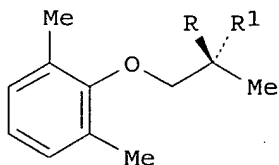
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

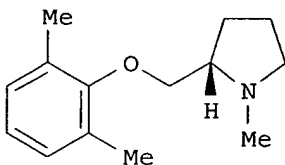
LANGUAGE: English

OTHER SOURCE(S): CASREACT 130:337878

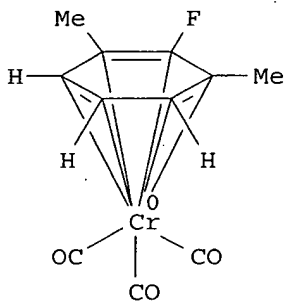
GI



I



II



III

AB Both enantiomers of mexiletine hydrochloride I (R = H₂N, H; R1 = H, H₂N) in addition to other racemic and nonracemic amine hydrochloride analogs such as II were prepared by nucleophilic aromatic substitution of the carbonylchromium complexed arene III with amino alcs. E.g., a solution of (S)-HOCH₂CH(NH₂)Me in THF was treated with sodium hydride dispersion and stirred, followed by the addition of III and stirring overnight. Iodine was

cautiously added, the mixture stirred for 2h, and the reaction washed with sodium bisulfite and sodium hydroxide to give upon workup the free base of (S)-mexiletine in 68% yield as an oily liquid which was treated with aqueous

HCl

in Et₂O to give (S)-(+)-mexiletine hydrochloride I (R = H₂N; R₁ = H, monohydrochloride salt) as a white solid in 41% yield.

L19 ANSWER 3 OF 13 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1998:668114. HCAPLUS

DOCUMENT NUMBER: 129:290061

TITLE: Phoxymethylpiperidine derivatives being sodium channel blockers

INVENTOR(S): Flippin, Lee Allen; Lin, Xiao-fa; Loughhead, David Garrett; Weikert, Robert James

PATENT ASSIGNEE(S): F. Hoffmann-La Roche A.-G., Switz.

SOURCE: Eur. Pat. Appl., 30 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

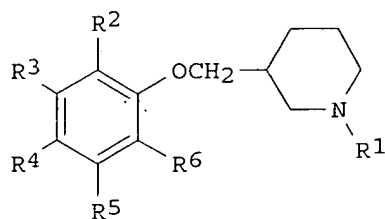
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 869119	A1	19981007	EP 1998-106026	19980402
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
CA 2232147	AA	19981003	CA 1998-2232147	19980316
AU 9859379	A1	19981008	AU 1998-59379	19980318
AU 743476	B2	20020124		
US 6110937	A	20000829	US 1998-46951	19980324
ZA 9802618	A	19981005	ZA 1998-2618	19980327
JP 10287649	A2	19981027	JP 1998-88372	19980401
JP 2938432	B2	19990823		
NO 9801495	A	19981005	NO 1998-1495	19980402
NO 310354	B1	20010625		
CN 1194977	A	19981007	CN 1998-106139	19980402
BR 9801225	A	19990601	BR 1998-1225	19980403
US 6262078	B1	20010717	US 2000-556130	20000420
PRIORITY APPLN. INFO.:			US 1997-42681P	P 19970403
			US 1997-69755P	P 19971216
			US 1997-66327P	P 19971121
			US 1998-46951	A3 19980324

OTHER SOURCE(S): MARPAT 129:290061

GI



AB The present invention relates to phoxymethyl piperidine derivs., and pharmaceutically acceptable salts and N-oxides thereof, which are Na

channel blockers, and thus exhibit useful pharmacol. properties, including utility for the treatment of neuropathic pain conditions. I were claimed, where is R1 is H, (C1-4)alkyl, -(CH2)mcyκλοalkyl, -(CH2)mNR7R8, or -(CH2)mNR7SO2R9; m is 1 to 3; R7 and R8 are independently H or (C1-4)alkyl; and R9 is (C1-4)alkyl; R2, R3, R5, and R6 are independently H, (C1-4)alkyl, or halogen; R4 is H, (C1-4)alkyl, hydroxy, alkyloxy, fluoroalkyloxy, halogen, or Ph or mono- or di-substituted Ph, the substituents selected from alkyloxy, amino, nitro or acetylamino; provided that when R1 is H at least two of R2, R3, R4, R5, and R6 are other than H; and further provided that when R1 is Me and R2, R3, R5 and R6 are H, R4 is other than fluoro; or a pharmaceutically acceptable salt or N-oxide thereof, as an individual isomer or as a racemic or nonracemic mixture of isomers. Thus, (S)-3-(4-bromo-2,6-dimethylphenoxy)methyl)piperidine (94.5 % yield) was prepared from (S)-N-(tert-butoxycarbonyl)-3-hydroxymethylpiperidine and 2,6-dimethylphenol followed by deprotection.

REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 4 OF 13 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1997:752748 HCAPLUS

DOCUMENT NUMBER: 128:39558

TITLE: Sodium channel blockers for the treatment of neuropathic pain

INVENTOR(S): Berger, Jacob; Flippin, Lee Allen; Hunter, John Cureton; Loughhead, David Garrett; Weikert, Robert James

PATENT ASSIGNEE(S): Syntex (U.S.A.) Inc., USA

SOURCE: U.S., 9 pp.
CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5688830	A	19971118	US 1997-782700	19970116
PRIORITY APPLN. INFO.:			US 1997-782700	19970116

AB This invention relates to [2-(2,6-dimethylphenoxy)-1-methylethyl]-ethylamine (I) as a racemic mixture and its individual enantiomers, in particular the (R)-enantiomer, and their pharmaceutically acceptable salts. These compds. are useful as sodium channel blockers, and are particularly useful for the alleviation of neuropathic pain. Various formulations containing (R)-I-HCl were provided.

L19 ANSWER 5 OF 13 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1997:525850 HCAPLUS

DOCUMENT NUMBER: 127:176263

TITLE: Preparation of N-[2-(2,6-dimethylphenoxy)-1-methylethyl]ethylamine as sodium channel blocker
INVENTOR(S): Berger, Jacob; Flippin, Lee Allen; Hunter, John Cureton; Loughhead, David Garrett; Weikert, Robert James

PATENT ASSIGNEE(S): F. Hoffmann-La Roche A.-G., Switz.

SOURCE: PCT Int. Appl., 37 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

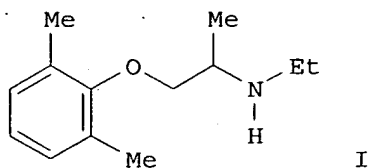
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9727169	A1	19970731	WO 1997-EP135	19970121
W: AL, AU, BA, BB, BG, BR, CA, CN, CZ, EE, GE, HU, IL, IS, JP, KP, KR, LK, LR, LT, LV, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, TR, TT, UA, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9714417	A1	19970820	AU 1997-14417	19970121
PRIORITY APPLN. INFO.:			US 1996-11048P	P 19960125
			WO 1997-EP135	W 19970121

GI



AB The title compound I, useful for the alleviation of neuropathic pain, was prepared by reaction of mexiletine.HCl with AcCl in the presence of 5N NaOH in EtOAc followed by treatment of the resulting N-[2-(2,6-dimethylphenoxy-1-methylethyl)]acetamide with BH₃*Me₂S in THF. Resolution of racemic compound I is also described. Compound (R)-I exhibited greater maximal analgesic activity (98% E_{max}) in vivo against mech. allodynia than rac-I (66% E_{max}). Pharmaceutical formulation of a tablet, capsule, suspension and topical formulation containing compound I was given.

L19 ANSWER 6 OF 13 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1997:450360 HCAPLUS

DOCUMENT NUMBER: 127:121589

TITLE: The florisisil catalyzed [1,3]-sigmatropic shift of allyl phenyl ethers - an entryway into novel mycophenolic acid analogs

AUTHOR(S): Talamas, Francisco X.; Smith, David B.; Cervantes, Alicia; Franco, Fidencio; Cutler, Serena T.; Loughhead, David G.; Morgans, David J., Jr.; Weikert, Robert J.

CORPORATE SOURCE: Division de Investigacion, Syntex, S. A. de C. V., Morelos, 62500, Mex.

SOURCE: Tetrahedron Letters (1997), 38(27), 4725-4728
CODEN: TELEAY; ISSN: 0040-4039

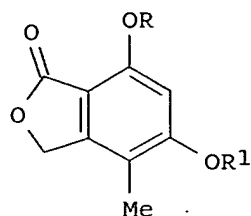
PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

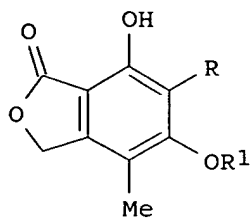
LANGUAGE: English

OTHER SOURCE(S): CASREACT 127:121589

GI



I



II

AB Florisil was found to be effective in promoting the [1,3]-sigmatropic shift of mycophenolic acid related allyl Ph ethers. Several novel mycophenolic acid analogs were thus prepared E.g., alkenyloxylactone I ($R = \text{CH}_2\text{CH:CMe}_2$, $R_1 = \text{CH}_3$) in toluene at 110° in the presence of Florisil underwent rearrangement to form the corresponding phenol II and dealkenylated product II ($R = \text{H}$) in 50:20 ratio. Through a crossover exptl. using two deuterated analogs I [$R = \text{CH}_2\text{CH:C}(\text{CD}_3)_2$, $R_1 = \text{CH}_3$; $R = \text{CH}_2\text{CH:CMe}_2$, $R_1 = \text{CD}_3$] of the model system, the reaction was shown to be intramol.

REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 7 OF 13 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1996:136169 HCAPLUS

DOCUMENT NUMBER: 124:260658

TITLE: Asymmetric Synthesis and Stereochemical Assignment of RS-97613, a Potent Immunosuppressive and Antiinflammatory Agent

AUTHOR(S): Smith, David B.; Waltos, Ann Marie; Loughhead, David G.; Weikert, Robert J.; Morgans, David J., Jr.; Rohloff, John C.; Link, John O.; Zhu, Rong-rong

CORPORATE SOURCE: Department of Medicinal Chemistry, Institute of Organic Chemistry, Palo Alto, CA, 94304, USA

SOURCE: Journal of Organic Chemistry (1996), 61(6), 2236-41
CODEN: JOCEAH; ISSN: 0022-3263

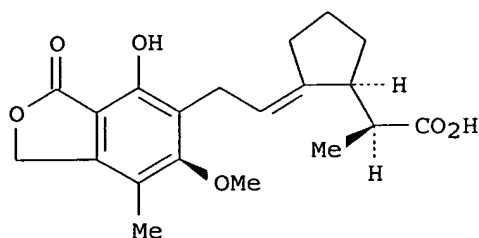
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

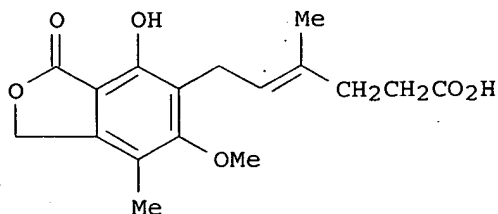
LANGUAGE: English

OTHER SOURCE(S): CASREACT 124:260658

GI



I



II

AB A practical asym. synthesis of RS-97613 (I), a potent inhibitor of inosine monophosphate dehydrogenase (IMPDH) is described. The synthesis begins with mycophenolic acid (II) and utilizes as key steps the coupling of cyclopentenylzinc chloride to an acid chloride, a modified CBS reduction of an achiral enone, a Johnson Claisen rearrangement, and a diastereoselective alkylation of an ester. The overall yield for the nine step sequence from II to I is 25%. Both the absolute and relative stereochem. of the compound have been unambiguously established. In vivo (mouse hemolytic plaque forming assay, rat adjuvant induced arthritis), the compound has proven to be more than 5 times as potent as mycophenolic acid (II) as an immunosuppressive and antiinflammatory agent.

L19 ANSWER 8 OF 13 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1995:485511 HCAPLUS

DOCUMENT NUMBER: 122:232909

TITLE: Photosynthetic performance, chloroplast pigments and mineral content of Norway spruce (*Picea abies* (L.) Karst.) exposed to SO₂ and O₃ in an open-air fumigation experiment

AUTHOR(S): Wedler, M.; Weikert, R. M.; Lippert, M.

CORPORATE SOURCE: Julius-von-Sachs-Institut Biowissenschaften, Botanik II, Universitaet Wuerzburg, Wuerzburg, 97082, Germany

SOURCE: Plant, Cell and Environment (1995), 18(3), 263-76

CODEN: PLCEDV; ISSN: 0140-7791

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Photosynthetic performance, mineral content and chloroplast pigments were investigated in August-Sept. 1988 and 1989 in Norway spruce trees (*Picea abies* (L.) Karst.) exposed to SO₂ and O₃ in an open-air fumigation facility at Liphook, England. The data do not suggest a treatment effect on the mineral content of the needles in terms of nutrient leaching from the foliage. In addition, there were no direct SO₂ and/or O₃ effects on the content and/or composition of the chloroplast pigments. However, the long-term application of SO₂ resulted in a depression of net photosynthesis under light saturation and ambient CO₂ (A340) which was probably caused by a treatment-related depression of the carboxylation efficiency (CE). In 1989, the supposed treatment effects were apparently masked by an

insufficient N-supply and probably also by low water availability during summer. However, fumigation appeared to accelerate an N-deficiency-related decrease of CE, stomatal closure and the age-dependent development of the chlorophyll content of the needles. In 1989, an observed depression of the photosynthetic capacity (A2500) was in part accompanied by a decrease in light use efficiency (α), suggesting an enhanced photosensitivity resulting from the impact of several possible interacting stresses (drought, N deficiency and fumigation). The results support the general conclusion that long-term low-level SO₂ dosage adversely affects the photosynthetic performance of the needle, whether directly or indirectly, and may also interact with other environmental stresses. The findings of the investigations are discussed with regard to the hypothesis of forest decline in the mountain regions of the Fichtelgebirge (north-eastern Bavaria, Germany).

L19 ANSWER 9 OF 13 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1992:128801 HCAPLUS

DOCUMENT NUMBER: 116:128801

TITLE: Novel benzothiophene-, benzofuran-, and naphthalenecarboxamidotetrazoles as potential antiallergy agents

AUTHOR(S): Connor, David T.; Cetenko, Wiaczeslaw A.; Mullican, Michael D.; Sorenson, Roderick J.; Unangst, Paul C.; Weikert, Robert J.; Adolphson, Richard L.; Kennedy, John A.; Thueson, David O.; et al.

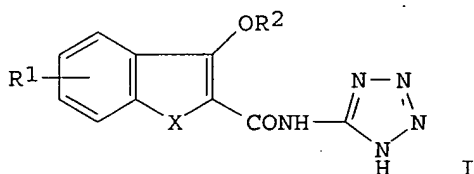
CORPORATE SOURCE: Dep. Chem., Parke-Davis Pharm. Res. Div., Ann Arbor, MI, 48105, USA

SOURCE: Journal of Medicinal Chemistry (1992), 35(5), 958-65
CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



AB The synthesis and antiallergic activity of a series of novel benzothiophene-, benzofuran-, and naphthalenecarboxamidotetrazoles I [R₁ = MeO, OH, Cl, NO₂, Me, H, PhO, PhCH₂O, 5,6-(MeO)₂, 6-MeO, 7-Cl; R₂ = alkyl, Ph, PhCH₂; X = S, O, CH:CH] are described. A number of the compds. inhibit the release of histamine from anti-IgE stimulated basophils obtained from allergic donors. Optimal inhibition is exhibited in benzothiophenes with a 3-alkoxy substituent in combination with a 5-methoxy, 6-methoxy, or a 5,6-dimethoxy group. Compound I (R₁ = 5-OMe, R₂ = Me₂CH, X = S) inhibited respiratory burst of human neutrophils and the release of mediators from anti-IgE-stimulated human chopped lung.

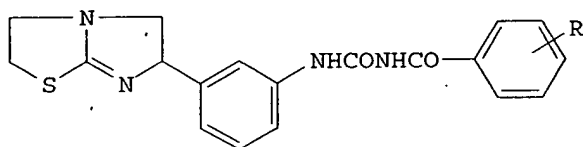
L19 ANSWER 10 OF 13 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1991:228822 HCAPLUS

DOCUMENT NUMBER: 114:228822

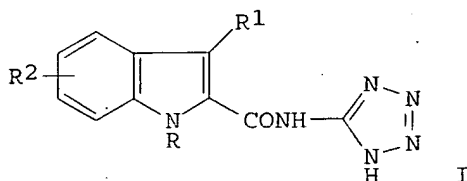
TITLE: Synthesis and anthelmintic activity of 3'-benzoylurea derivatives of 6-phenyl-2,3,5,6-tetrahydroimidazo[2,1-b]thiazole

AUTHOR(S): Weikert, Robert J.; Bingham, Stanford, Jr.; Emanuel, Mark A.; Fraser-Smith, Elizabeth B.; Loughhead, David G.; Nelson, Peter H.; Poulton, Anthony L.
 CORPORATE SOURCE: Inst. Org. Chem., Syntex Res., Palo Alto, CA, 94304, USA
 SOURCE: Journal of Medicinal Chemistry (1991), 34(5), 1630-3
 CODEN: JMCMAR; ISSN: 0022-2623
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 114:228822
 GI



AB Reaction of 3-amino derivs. of the nematocides tetramisole and levamisole with variously substituted benzoyl isocyanates gave a series of benzoylureas (I; R = 2-, 4-OMe, 2-, 3-, 4-NO₂, 4-OCF₃, 4-CN, 2-, 4-F, H, 4-I, 4-Bz, 3,5-, 2,6-F₂, 2-, 4-Cl, 4-CMe₃, 2,6-Cl₂) which were tested for activity against helminths and ectoparasites. Compds. bearing 2,6-difluoro and 4-trifluoromethyl substituents had potent nematocidal activity in both mice and sheep. No antiectoparasitic activity was observed

L19 ANSWER 11 OF 13 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1989:407305 HCAPLUS
 DOCUMENT NUMBER: 111:7305
 TITLE: Novel indolecarboxamidotetrazoles as potential antiallergy agents
 AUTHOR(S): Unangst, Paul C.; Connor, David T.; Stabler, S. Russell; Weikert, Robert J.; Carethers, Mary E.; Kennedy, John A.; Thueson, David O.; Chestnut, James C.; Adolphson, Richard L.; Conroy, M. C.
 CORPORATE SOURCE: Dep. Chem., Parke-Davis Pharm. Res. Div., Ann Arbor, MI, 48105, USA
 SOURCE: Journal of Medicinal Chemistry (1989), 32(6), 1360-6
 CODEN: JMCMAR; ISSN: 0022-2623
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 111:7305
 GI



AB The synthesis and antiallergic potential of a series of novel indolecarboxamidotetrazoles I [R = Ph, H, 4-MeOC₆H₄, Me, CH₂Ph; R₁ = OH, OMe, OEt, OCHMe₂, O(CH₂)₈Me, H, CHMe₂, SMe, SO₂Me, SCHMe₂, SPh, OC₆H₄NO₂-4; R₂ = 4-, 5-, 6-OMe, 5-OH, 5-OCH₂Ph, 5-Me, 5-Br, 5-Cl] is described. A number of compds. inhibit the release of histamine from anti-IgE-stimulated basophilic leukocyte obtained from allergic donors. Optimal inhibition is exhibited by compds. with 3-alkoxy, 5-methoxy, and 1-Ph substituents on the indole core structure. I (R = Ph, R₁ = OCHMe₂, R₂ = 5-OMe), designated CI-949, is a potent inhibitor of histamine release from human basophils and from guinea pig and human chopped lung.

L19 ANSWER 12 OF 13 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1988:631035. HCAPLUS

DOCUMENT NUMBER: 109:231035

TITLE: Preparation and testing of N-tetrazol-5-yl-2-naphthalenecarboxamides as histamine release inhibitors

INVENTOR(S): Connor, David Thomas; Unangst, Paul Charles; Weikert, Robert James

PATENT ASSIGNEE(S): Warner-Lambert Co., USA

SOURCE: Eur. Pat. Appl., 21 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

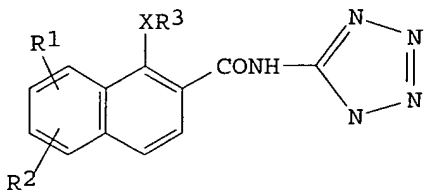
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 279466	A2	19880824	EP 1988-102487	19880219
EP 279466	A3	19890802		
EP 279466	B1	19930519		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
US 4767776	A	19880830	US 1987-16811	19870220
ZA 8800385	A	19890927	ZA 1988-385	19880120
AU 8811119	A1	19880901	AU 1988-11119	19880128
AU 596054	B2	19900412		
FI 8800748	A	19880821	FI 1988-748	19880217
DK 8800840	A	19880821	DK 1988-840	19880218
NO 8800731	A	19880822	NO 1988-731	19880219
JP 63222161	A2	19880916	JP 1988-35430	19880219
AT 89556	E	19930615	AT 1988-102487	19880219
ES 2054715	T3	19940816	ES 1988-102487	19880219
PRIORITY APPLN. INFO.:			US 1987-16811	A 19870220
			EP 1988-102487	A 19880219

OTHER SOURCE(S): CASREACT 109:231035; MARPAT 109:231035

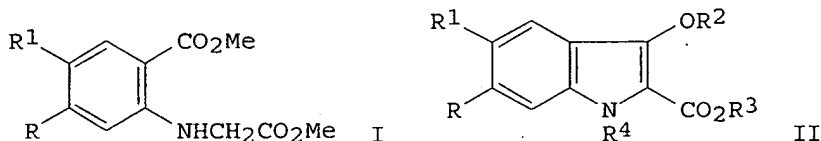
GI



AB The title compds. (I; R₁, R₂ = H, alkyl, alkoxy, SH, halo, OH, CF₃,

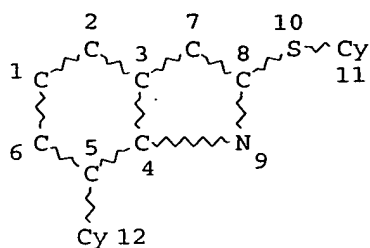
alkylthio, alkylsulfinyl, alkylsulfonyl, NO₂, amino; R₁R₂ = methylenedioxy; R₃ = C₁-12 alkyl; X = O, S) and their pharmaceutically acceptable salts were prepared as allergy and inflammation inhibitors. 6-Methoxy-1-(1-methylethoxy)-2-naphthalenecarboxylic acid and 1,1'-carbonyldiimidazole were refluxed 1 h in MeCN and 5-aminotetrazole and Et₃N were added. The mixture was refluxed for an addnl. 5 h to give 97% 6-methoxy-1-(1-methylethoxy)-N-1H-tetrazol-5-yl-2-naphthalenecarboxamide. At 33 μM I gave 16-91% inhibition of histamine release from human basophils in vitro.

L19 ANSWER 13 OF 13 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1988:131497 HCAPLUS
 DOCUMENT NUMBER: 108:131497
 TITLE: Synthesis of novel 1-phenyl-1H-indole-2-carboxylic acids. I. Utilization of Ullmann and Dieckmann reactions for the preparation of 3-hydroxy, 3-alkoxy, and 3-alkyl derivatives
 AUTHOR(S): Unangst, Paul C.; Connor, David T.; Stabler, S. Russell; Weikert, Robert J.
 CORPORATE SOURCE: Dep. Chem., Warner-Lambert/Parke-Davis Pharm. Res., Ann Arbor, MI, 48105, USA
 SOURCE: Journal of Heterocyclic Chemistry (1987), 24(3), 811-15
 CODEN: JHTCAD; ISSN: 0022-152X
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 108:131497
 GI



AB Methods for the synthesis of novel 3-hydroxy, 3-alkoxy, and 3-alkyl indole-2-carboxylic acids and esters are described. Dieckmann cyclization of various 2-[(carboxymethyl)amino]benzoic acid diesters yielded 1-unsubstituted-, 1-methyl-, and 1-phenyl-3-hydroxy-1H-indole-2-carboxylic acid esters. An Ullmann reaction with bromobenzene converted 1H-indoles to 1-phenylindoles. Thus, Dieckmann cyclization of benzoic acid diesters I (R = H, R₁ = OMe, Br; R = R₁ = Cl) gave indole esters II (R₂ = H, R₃ = Me, R₄ = H), which on alkylation with Me₂CHBr gave II (R₂ = CHMe₂). Ullmann reaction in PhBr as solvent and reagent converted II (R₂ = CHMe₂, R₃ = Me, R₄ = H) to II (R₂ = CHMe₂, R₃ = Me, R₄ = Ph) which upon saponification gave II (R₂ = CHMe₂, R₃ = H, R₄ = Ph).

=> => d stat que 130
 L10 STR

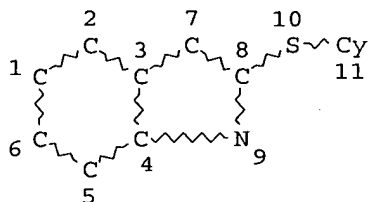


NODE ATTRIBUTES:
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 12

STEREO ATTRIBUTES: NONE

L12 22 SEA FILE=REGISTRY SSS FUL L10
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 L16 7 SEA FILE=HCAPLUS ABB=ON PLU=ON "MADERA A"/AU OR "MADERA ANN
 MARIE"/AU
 L17 6 SEA FILE=HCAPLUS ABB=ON PLU=ON L16 NOT L13
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 ROBERT J"/AU OR "WEIKERT ROBERT JAMES"/AU)
 L19 13 SEA FILE=HCAPLUS ABB=ON PLU=ON L18 NOT (L13 OR L17)
 L23 STR



NODE ATTRIBUTES:
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 11

STEREO ATTRIBUTES: NONE

L25 2001 SEA FILE=REGISTRY SSS FUL L23
 L26 STR

Hy~Hy~S~Cy
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NODE ATTRIBUTES:
 DEFAULT MLEVEL IS ATOM
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 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 4

STEREO ATTRIBUTES: NONE

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L28 38 SEA FILE=REGISTRY ABB=ON PLU=ON L27 NOT L12
L29 7 SEA FILE=HCAPLUS ABB=ON PLU=ON L28
L30 5 SEA FILE=HCAPLUS ABB=ON PLU=ON L29 NOT (L13 OR L17 OR L19)

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=> d ibib abs hitstr l30 1-5

L30 ANSWER 1 OF 5 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:470334 HCAPLUS

DOCUMENT NUMBER: 143:125834

TITLE: A Three-Dimensional Pharmacophore Model for
5-Hydroxytryptamine6 (5-HT6) Receptor Antagonists
AUTHOR(S): Lopez-Rodriguez, Maria L.; Benhamu, Bellinda; de la
Fuente, Tania; Sanz, Arantxa; Pardo, Leonardo;
Campillo, Mercedes

CORPORATE SOURCE: Departamento de Quimica Organica I, Facultad de
Ciencias Quimicas, Universidad Complutense, Madrid,
E-28040, Spain

SOURCE: Journal of Medicinal Chemistry (2005), 48(13),
4216-4219

CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Forty-five structurally diverse 5-hydroxytryptamine6 receptor (5-HT6R)
antagonists were selected to develop a 3D pharmacophore model with the
Catalyst software. The structural features for antagonism at this
receptor are a pos. ionizable atom interacting with Asp3.32, a hydrogen
bond acceptor group interacting with Ser5.43 and Asn6.55, a hydrophobic
site interacting with residues in a hydrophobic pocket between
transmembranes 3, 4, and 5, and an aromatic-ring hydrophobic site interacting
with Phe6.52.

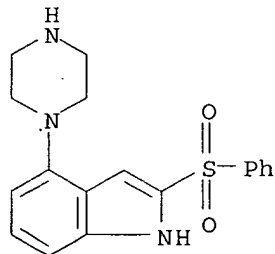
IT 676448-24-1

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
(Biological study); USES (Uses)

(three-dimensional pharmacophore model for 5-HT6 receptor antagonists)

RN 676448-24-1 HCAPLUS

CN 1H-Indole, 2-(phenylsulfonyl)-4-(1-piperazinyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 2 OF 5 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:41121 HCAPLUS

DOCUMENT NUMBER: 140:94045

TITLE: Preparation of hypoglycemic imidazoline compounds

INVENTOR(S): Takeuchi, Kumiko; Jirousek, Michael Robert; Paal, Michael; Ruhter, Gerd; Schotten, Theo

PATENT ASSIGNEE(S): USA

SOURCE: U.S. Pat. Appl. Publ., 106 pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent

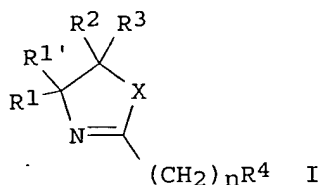
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004009976	A1	20040115	US 2002-135963	20020430
PRIORITY APPLN. INFO.:			US 2002-135963	20020430
OTHER SOURCE(S):	MARPAT	140:94045		

GI



AB The title compds. I [X = O, S, NR₅ with R₅ = H, alkyl, protecting group; R₁, R₁', R₂, R₃ = H, alkyl; R₁ and R₂ form a bond and R₁' and R₃ are H, alkyl; or R₁ and R₂ form a carbocyclic ring; R₄ = (un)substituted indolyl, naphthyl, quinolinyl, etc.; n = 0-2], useful for treating diabetes, diabetic complications, metabolic disorders or related diseases where impaired glucose disposal is present, were prepared and formulated. E.g., preparation of 5-chloro-2-methyl-3-(4,5-dihydro-1H-imidazol-2-yl)-1H-indole is described.

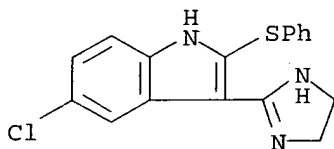
IT 227800-70-6P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of hypoglycemic imidazolines)

RN 227800-70-6 HCAPLUS

CN 1H-Indole, 5-chloro-3-(4,5-dihydro-1H-imidazol-2-yl)-2-(phenylthio)- (9CI)
(CA INDEX NAME)



L30 ANSWER 3 OF 5 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:521746 HCAPLUS

DOCUMENT NUMBER: 137:93770

TITLE: Preparation of tricyclic spiro compounds and cholesterol biosynthesis inhibitors containing them as the active ingredient

INVENTOR(S): Nishida, Hidemitsu; Mukaihira, Takafumi

PATENT ASSIGNEE(S): Mochida Pharmaceutical Co., Ltd., Japan

SOURCE: PCT Int. Appl., 311 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

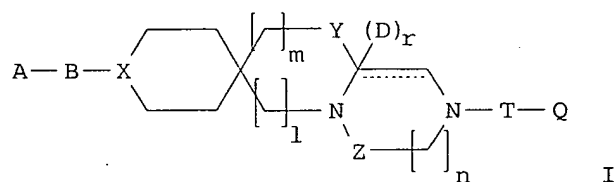
FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002053568	A1	20020711	WO 2001-JP11656	20011228
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG CA 2433174 AA 20020711 CA 2001-2433174 20011228 EP 1346994 A1 20030924 EP 2001-272922 20011228 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR US 2004063716 A1 20040401 US 2003-451728 20030625 PRIORITY APPLN. INFO.: JP 2000-399998 A 20001228 WO 2001-JP11656 W 20011228				

OTHER SOURCE(S): MARPAT 137:93770

GI



AB Disclosed are orally administrable cholesterol biosynthesis inhibitors and oxidosqualene cyclase inhibitors which contain as the active ingredients tricyclic spiro compds., i.e. 1,4-diaza-7-oxaspiro[bicyclo[4.3.0]nonane-8,4'-piperidine]-2-one and 1,4,7-triazaspiro[bicyclo[4.3.0]nonane-8,4'-piperidine]-2-one derivs. represented by the general formula (I) or salts thereof: [wherein A = H, (un)substituted 5- or 6-membered (un)saturated heterocyclic or carbocyclic group, (un)substituted NH₂ or imidoyl; B = a single bond, carbonyl, S(O)_x (x = 0,1,2), C1-2 alkylene; D = H, COR₅ (R₅ = H, substituent), (un)substituted C1-6 alkyl; X = N, CH optionally substituted by A'-B' group (A' and B' are selected from groups defined in A and B, resp.); Y = O, S(O)_y (y = 0,1,2), NH; Z = CH₂, CO, C(:S); T =

SO₂, CO, S(O)_z (z = 0,1,2), a single bond, (un)substituted C1-2 alkylene; Q = (un)substituted hydrocarbon or heterocyclic group; m, n, p = 0,1, or 2, provided that m and p are not simultaneously 0; q = 0,1; each of 3 rings cong. X, Y, and Z is optionally substituted; the solid line accompanied by a dotted line represents a single bond or a double bond when q is 0]. These compds. inhibit oxidosqualene cyclase and in turn the conversion of 2,3-oxidosqualene into cholesterol and thereby exhibit potent serum cholesterol lowering effect and are useful for the prevention and/or treatment of cholesterol biosynthesis and oxidosqualene cyclase-related diseases such as hypercholesteremia, hyperlipidemia, arteriosclerotic disease, myocardial infarction, angina pectoris, cerebral infarction, cerebral hemorrhage, aortic aneurysm, peripheral artery obstruction, nephrosclerosis, optic nerve atrophy, hydrocephalus, and fungal infection. Thus, Et₃N and 4-bromobenzenesulfonyl chloride were added to a soln. of 1,4-diaza-4-(benzyloxycarbonyl)-7-oxaspiro[bicyclo[4.3.0]nonane-8,4'-piperidine]-2-one in CH₂Cl₂ and stirred at room temperature for 10 min to give 1,4-diaza-4-(benzyloxycarbonyl)-1'-(4-bromobenzenesulfonyl)-7-oxaspiro[bicyclo[4.3.0]nonane-8,4'-piperidine]-2-one which was dissolved in MeCN, treated with trimethylsilyl iodide under ice-cooling, and stirred for 30 min under ice-cooling to give 1,4-diaza-1'-(4-bromobenzenesulfonyl)-7-oxaspiro[bicyclo[4.3.0]nonane-8,4'-piperidine]-2-one (II). II at 0.3 µg/mL in vitro inhibited the biosynthesis of cholesterol in mouse fibroblast L929 cells by 66%.

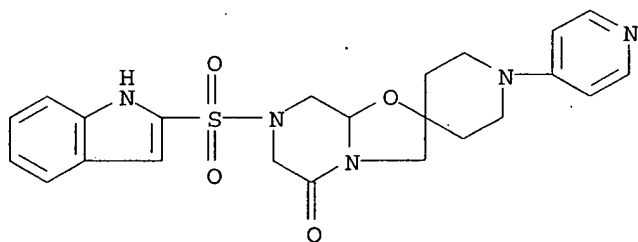
IT 441789-00-0P 441791-07-7P 441791-08-8P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of tricyclic spiro compds. as oxidosqualene cyclase inhibitors and cholesterol biosynthesis inhibitors for preventives and therapeutic agents)

RN 441789-00-0 HCAPLUS

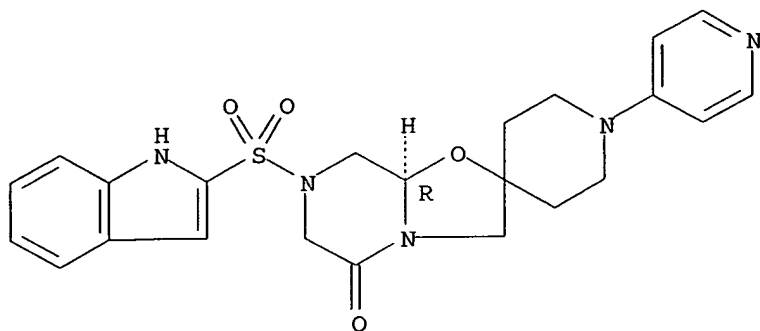
CN Spiro[5H-oxazolo[3,2-a]pyrazine-2(3H),4'-piperidin]-5-one, tetrahydro-7-(1H-indol-2-ylsulfonyl)-1'-(4-pyridinyl)- (9CI) (CA INDEX NAME)



RN 441791-07-7 HCAPLUS

CN Spiro[5H-oxazolo[3,2-a]pyrazine-2(3H),4'-piperidin]-5-one, tetrahydro-7-(1H-indol-2-ylsulfonyl)-1'-(4-pyridinyl)-, (8aR)- (9CI) (CA INDEX NAME)

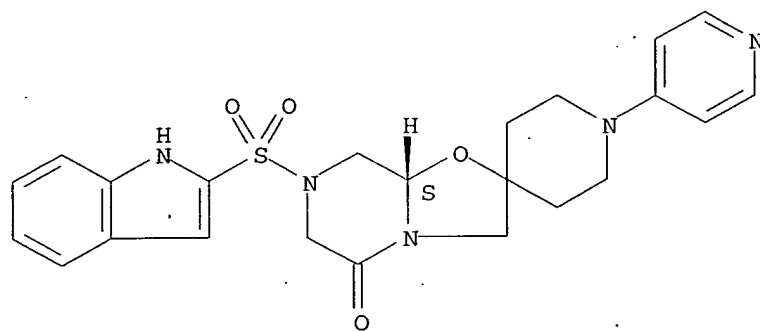
Absolute stereochemistry.



RN 441791-08-8 HCAPLUS

CN Spiro[5H-oxazolo[3,2-a]pyrazine-2(3H),4'-piperidin]-5-one,
tetrahydro-7-(1H-indol-2-ylsulfonyl)-1'-(4-pyridinyl)-, (8aS)- (9CI) (CA
INDEX NAME)

Absolute stereochemistry.



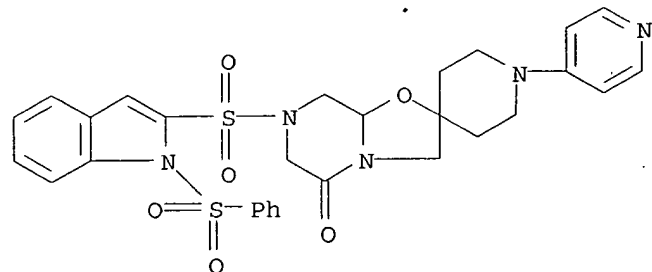
IT 441790-40-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)

(preparation of tricyclic spiro compds. as oxidosqualene cyclase inhibitors
and cholesterol biosynthesis inhibitors for preventives and therapeutic
agents)

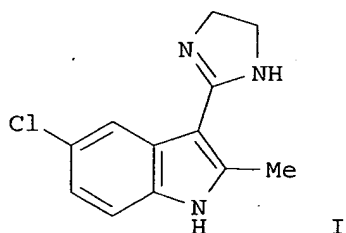
RN 441790-40-5 HCAPLUS

CN Spiro[5H-oxazolo[3,2-a]pyrazine-2(3H),4'-piperidin]-5-one,
tetrahydro-7-[[1-(phenylsulfonyl)-1H-indol-2-yl]sulfonyl]-1'-(4-pyridinyl)-
(9CI) (CA INDEX NAME)

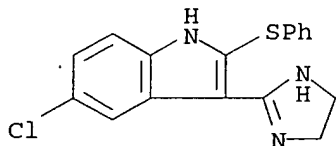


REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 4 OF 5 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 2001:501900 HCAPLUS
 DOCUMENT NUMBER: 135:303820
 TITLE: Efficient synthesis of 3-(4,5-dihydro-1H-imidazol-2-yl)-1H-indoles
 AUTHOR(S): Hary, U.; Roettig, U.; Paal, M.
 CORPORATE SOURCE: Lilly Forschung GmbH, Hamburg, 22419, Germany
 SOURCE: Tetrahedron Letters (2001), 42(31), 5187-5189
 CODEN: TELEAY; ISSN: 0040-4039
 PUBLISHER: Elsevier Science Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 135:303820
 GI



AB A simple method for the synthesis of various 3-(4,5-dihydro-1H-imidazol-2-yl)-1H-indoles, e.g. I, is described. Treatment of different substituted indoles with 1-acetylimidazolidin-2-one in the presence of phosphorus oxychloride afforded after hydrolysis in ethanol the corresponding 3-(4,5-dihydro-1H-imidazol-2-yl)-1H-indoles in moderate to good yields.
 IT 227800-70-6P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of imidazolyloindoles by coupling of indoles with acetylimidazolidinone)
 RN 227800-70-6 HCAPLUS
 CN 1H-Indole, 5-chloro-3-(4,5-dihydro-1H-imidazol-2-yl)-2-(phenylthio)- (9CI)
 (CA INDEX NAME)



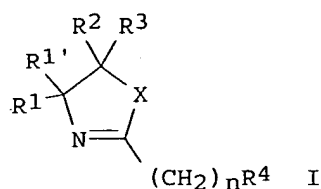
REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 5 OF 5 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1999:401581 HCAPLUS
 DOCUMENT NUMBER: 131:58827
 TITLE: Preparation of hypoglycemic imidazoline compounds
 INVENTOR(S): Jirousek, Michael Robert; Paal, Michael; Ruhter, Gerd;

PATENT ASSIGNEE(S): Schotten, Theo; Stenzel, Wolfgang; Takeuchi, Kumiko
 SOURCE: Eli Lilly and Co., USA
 Eur. Pat. Appl., 136 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 924209	A1	19990623	EP 1998-310461	19981218
EP 924209	B1	20030502		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
CA 2315226	AA	19990701	CA 1998-2315226	19981218
WO 9932112	A1	19990701	WO 1998-US26974	19981218
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RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
WO 9932482	A1	19990701	WO 1998-US27080	19981218
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RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 9920030	A1	19990712	AU 1999-20030	19981218
AU 9922016	A1	19990712	AU 1999-22016	19981218
ZA 9811672	A	20000619	ZA 1998-11672	19981218
JP 2001526286	T2	20011218	JP 2000-525419	19981218
EP 1266897	A2	20021218	EP 2002-20546	19981218
EP 1266897	A3	20031203		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, SI, LT, LV, FI, RO, CY, AL				
AT 239013	E	20030515	AT 1998-310461	19981218
PT 924209	T	20030829	PT 1998-310461	19981218
ES 2198033	T3	20040116	ES 1998-310461	19981218
US 6410562	B1	20020625	US 2000-581498	20001208
PRIORITY APPLN. INFO.:				
			US 1997-68195P	P 19971219
			EP 1998-310461	A3 19981218
			WO 1998-US26974	W 19981218
			WO 1998-US27080	W 19981218

OTHER SOURCE(S): MARPAT 131:58827
 GI

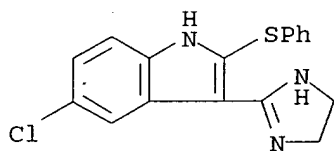


AB The title compds. I [X = O, S, NR₅ with R₅ = H, alkyl, protecting group; R₁, R₁', R₂, R₃ = H, alkyl; R₁ and R₂ form a bond and R₁' and R₃ are H, alkyl; R₁ and R₂ form a carbocyclic ring; R₄ = heterocyclyl; n = 0-2], hypoglycemic agents, were prepared E.g., 5-chloro-2-methyl-3-(4,5-dihydro-1H-imidazol-2-yl)-1H-indole was prepared

IT 227800-70-6P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of hypoglycemic imidazoline compds.)

RN 227800-70-6 HCAPLUS

CN 1H-Indole, 5-chloro-3-(4,5-dihydro-1H-imidazol-2-yl)-2-(phenylthio)- (9CI)
 (CA INDEX NAME)



REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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Ward 10_663314 - - History

=> d his ful

(FILE 'REGISTRY' ENTERED AT 16:10:16 ON 07 APR 2006)

FILE 'REGISTRY' ENTERED AT 16:27:39 ON 07 APR 2006

L10 STR
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FILE 'HCAPLUS' ENTERED AT 16:31:36 ON 07 APR 2006

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D STAT QUE L13
D IBIB ABS HITSTR L13 1-2

FILE 'BEILSTEIN' ENTERED AT 16:32:52 ON 07 APR 2006

L14 1 SEA SSS FUL L10
L15 1 SEA ABB=ON PLU=ON L14 NOT L12
D STAT QUE L15
D BRN CN MF FW BSO STR RX 1

FILE 'HCAPLUS' ENTERED AT 16:33:55 ON 07 APR 2006

L16 7 SEA ABB=ON PLU=ON "MADERA A"/AU OR "MADERA ANN MARIE"/AU
L17 6 SEA ABB=ON PLU=ON L16 NOT L13
D STAT QUE L17
D IBIB ABS L17 1-6
L18 18 SEA ABB=ON PLU=ON ("WEIKERT R M"/AU OR "WEIKERT ROBERT J"/AU
OR "WEIKERT ROBERT JAMES"/AU)
L19 13 SEA ABB=ON PLU=ON L18 NOT (L13 OR L17)
D STAT QUE L19
D IBIB ABS HITSTR L19 1-13

FILE 'REGISTRY' ENTERED AT 16:36:54 ON 07 APR 2006

L23 STR
L25 2001 SEA SSS FUL L23
L26 STR
L27 60 SEA SUB=L25 SSS FUL L26
L28 38 SEA ABB=ON PLU=ON L27 NOT L12

FILE 'HCAPLUS' ENTERED AT 16:39:31 ON 07 APR 2006

L29 7 SEA ABB=ON PLU=ON L28
L30 5 SEA ABB=ON PLU=ON L29 NOT (L13 OR L17 OR L19)
D STAT QUE L30
D IBIB ABS HITSTR L30 1-5

FILE REGISTRY

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 5 APR 2006 HIGHEST RN 879397-30-5
DICTIONARY FILE UPDATES: 5 APR 2006 HIGHEST RN 879397-30-5

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

*

*

Ward 10_663314 - - History

* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
*

Structure search iteration limits have been increased. See HELP SLIMITS for details.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

FILE HCAPLUS

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FILE COVERS 1907 - 7 Apr 2006 VOL 144 ISS 16
FILE LAST UPDATED: 6 Apr 2006 (20060406/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

FILE BEILSTEIN
FILE LAST UPDATED ON MARCH 15, 2006

FILE COVERS 1771 TO 2006.
FILE CONTAINS 9,516,393 SUBSTANCES

>>>PLEASE NOTE: Reaction Data and substance data are stored in separate documents and can not be searched together in one query. Reaction data for BEILSTEIN compounds may be displayed immediately with the display codes PRE (preparations) and REA (reactions). A substance answer set retrieved after the search for a chemical name, a compounds with available reaction information by combining with PRE/FA, REA/FA or more generally with RX/FA. The BEILSTEIN Registry Number (BRN) is the link between a BEILSTEIN compound and belonging reactions. For more detailed reaction searches BRNs can be searched as reaction partner BRNs Reactant BRN (RX.RBRN) or Product BRN (RX.PBRN).<<<

>>> FOR SEARCHING PREPARATIONS SEE HELP PRE <<<

* PLEASE NOTE THAT THERE ARE NO FORMATS FREE OF COST. *
* SET NOTICE FEATURE: THE COST ESTIMATES CALCULATED FOR SET NOTICE *

Ward 10_663314 - - History

* ARE BASED ON THE HIGHEST PRICE CATEGORY. THEREFORE; THESE *
* ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS. *
* FOR PRICE INFORMATION SEE HELP COST *

NEW

* PATENT NUMBERS (PN) AND BABS ACCESSION NUMBERS (BABSAN) CAN NOW BE
SEARCHED, SELECTED AND TRANSFERRED.
* NEW DISPLAY FORMATS ALLREF, ALLP AND BABSAN SHOW ALL REFERENCES,
ALL PATENT REFERENCES, OR ALL BABS ACCESSION NUMBERS FOR A
COMPOUND AT A GLANCE.

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